Complex Eigenvalues of
the Parabolic Potential Barrier
and Gel'fand Triplet

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Abstract

The paper deals with the one-dimensional parabolic potential barrier $V(x) = V_0 - m\gamma^2 x^2/2$, as a model of an unstable system in quantum mechanics. The time-independent Schrödinger equation for this model is set up as the eigenvalue problem in Gel'fand triplet and its exact solutions are expressed by generalized eigenfunctions belonging to complex energy eigenvalues $V_0 \mp i\Gamma_n$ whose imaginary parts are quantized as $\Gamma_n = (n + 1/2)\hbar\gamma$. Under the assumption that time factors of an unstable system are square integrable, we provide a probabilistic interpretation of them. This assumption leads to the separation of the domain of the time evolution, namely all the time factors belonging to the complex energy eigenvalues $V_0 - i\Gamma_n$ exist on the future part and all those belonging to the complex energy eigenvalues $V_0 + i\Gamma_n$ exist on the past part. In this model the physical energy distributions worked out from these time factors are found to be the Breit-Wigner resonance formulas. The half-widths of these physical energy distributions are determined by the imaginary parts of complex energy eigenvalues, and hence they are also quantized.

1   Introduction

It is well known that time-dependent wave functions of non-relativistic quantum mechanics satisfy the time-dependent Schrödinger equation

$$i\hbar\frac{\partial}{\partial t}\psi(t,q) = \hat{H}\psi(t,q), \tag{1.1}$$

where $\hat{H}$ is the Hamiltonian of the system expressed in the coordinate representation. According to Born's probabilistic interpretation, the square of modulus of a time-dependent wave function $\psi(t,q)$ multiplied by a small volume Δq of the coordinate space,

$$|\psi(t,q)|^2\,\Delta q \tag{1.2}$$

is the relative probability of the particle being within the small volume Δq of the point q at the time t. If the time-dependent wave function $\psi(t,q)$ is normalized,

$$\int |\psi(t,q)|^2\,dq = 1, \tag{1.3}$$

then the formula (1.2) gives directly the probability. In this case the expectation value of any observable $\hat{O}$ is

$$\langle O \rangle_t = \int \psi(t,q)^*\hat{O}\psi(t,q)dq, \tag{1.4}$$

which is a function of t. When a potential energy does not involve the time t explicitly, we can separate variables of a time-dependent wave function

$$\psi(t,q) = T(t)u(q). \tag{1.5}$$

For the state of a energy eigenvalue E, the time factor $T(t)$ is of the form

$$T(t) = Ae^{-iEt/\hbar}, \tag{1.6}$$

where $A \in \mathbb{C}$ is independent of t, and equation (1.1) for it reduces to the time-independent Schrödinger equation

$$\hat{H}u(q) = Eu(q). \tag{1.7}$$

In the case when the energy eigenvalue E of (1.7) is a real number, the formula (1.2) will reduce to

$$|u(q)|^2\,\Delta q, \tag{1.8}$$

where $u(q)$ contains A as a numerical coefficient. We then have, instead of (1.3)

$$\int |u(q)|^2\,dq = 1, \tag{1.9}$$

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and instead of (1.4) we get

$$\langle O \rangle_t = \int u(q)^* \hat{O} u(q) dq. \tag{1.10}$$

Thus the probability is independent of the time. We call a state belonging to the real energy eigenvalue a *stationary state* [1, 2, 3]. If we cannot normalize an eigenfunction $u(q)$, we obtain the expectation value of $\hat{O}$, as the generalization of (1.10)

$$\langle O \rangle_t = \int u(q)^* \hat{O} u(q) dq \Big/ \int |u(q)|^2 \, dq. \tag{1.10'}$$

However, the energy eigenvalue E can be a complex number for an unstable system in which the potential energy do not have a stable stationary point. The eigenfunction $u(q)$ of the Hamiltonian $\hat{H}$ belonging to the complex energy eigenvalue is not expressible in terms of the vector of a Hilbert space, since $\hat{H}$ is a self-adjoint operator on a Hilbert space. The problems of the mathematical formulations of continuous spectrum or complex eigenvalues has been treated by Bohm and Gadella [4] on the basis of a *rigged Hilbert space* or a *Gel'fand triplet* [5]. They suggested by the analysis of S-matrices that the states belonging to continuous spectrum or complex eigenvalues are expressible in terms of the *generalized functions* of a Gel'fand triplet, and their time evolution associates with a one-parameter semigroup.

The object of the present paper is to show that the exact solution of the time-independent Schrödinger equation (1.7) for an unstable potential energy becomes the generalized function belonging to the complex energy eigenvalue. As a model Hamiltonian of the unstable system, we take the one-dimensional parabolic potential barrier. The collision problem of this model Hamiltonian was first solved by Kemble [6] by the method of the WKB approximation. We consider the eigenvalue problem of this model Hamiltonian in § 2 at one instant of time. In § 2.1 this problem is worked out in the coordinate representation. We show that the energy eigenvalues are complex numbers and the corresponding eigenfunctions are expressible in terms of the generalized functions of a Gel'fand triplet. In § 2.2 the same problem is dealt with in the momentum representation.

Physically these complex eigenvalues play an important part in the resonance scattering. Since a state of resonance is only approximately stationary, its mean lifetime will be finite. This means the probability of the particle being inside the system tends to zero after a sufficient lapse of time, and the generalized eigenfuction $u(q)$ remains finite at $|q| \to \infty$. This is a physical reason why $u(q)$ is not expressible in a Hilbert vector and does not satisfy the normalizing condition (1.9). Such a state is called a *non-stationary state* [1, 3] or a *quasi-stationary state* [2]. Let us now try to assume the normalizing condition for the time factor

$$\int |T(t)|^2 \, dt = 1, \tag{1.11}$$

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since the mean lifetime of the non-stationary state is finite. This condition will be seen later (see § 3.2) to be connected with the fact that the Breit-Wigner resonance formula is normalized. We can now proceed to introduce a physical interpretation of the time factor $T(t)$ such that the absolute probability of the particle being during the time interval t to $t + \Delta t$ is given by

$$|T(t)|^2 \, \Delta t. \tag{1.12}$$

This interpretation provides a physical description of a process of time for a non-stationary state, say from growth to decay. When this interpretation is adapted to Born's one, the square of modulus of $\psi(t, q)$ corresponding to a non-stationary state, multiplied by $\Delta t \Delta q$,

$$|\psi(t, q)|^2 \, \Delta t \Delta q \tag{1.13}$$

gives the relative probability of the particle being within the small volume Δq of the point q during the time interval t to $t + \Delta t$. The time average of the expectation value of $\hat{O}$ will be

$$\langle O \rangle = \iint \psi(t, q)^* \hat{O} \psi(t, q) dt dq \Big/ \int |u(q)|^2 \, dq \tag{1.14}$$

as the generalization of $(1.10')$.

In § 3 the motion of the unstable system consisting of the one-dimensional parabolic potential barrier is considered. The above theory is applied to this motion in § 3.1. In § 3.2 it is shown that the connection between the physical energy distributions and the complex energy eigenvalues given by § 2.1.

2 Eigenvalue problems of the parabolic potential barrier

2.1 The coordinate representation

A simple and interesting model of an unstable system in quantum mechanics is the one-dimensional parabolic potential barrier. The Hamiltonian in quantum mechanics is

$$\hat{H} = -\frac{\hbar^2}{2m} \frac{d^2}{dx^2} + V_0 - \frac{1}{2} m \gamma^2 x^2, \tag{2.1}$$

where $V_0 \in \mathbb{R}$ is the maximum potential energy, $m > 0$ is the mass and $\gamma > 0$ is proportional to the square root of the curvature at $x = 0$. This Hamiltonian can be obtained from the Hamiltonian of the harmonic oscillator (A.1) with the replacement

$$\omega \to \mp i\gamma. \tag{2.2}$$

Thus $\hat{H}$ is an essentially self-adjoint on a Schwartz space $\mathcal{S}(\mathbb{R}_x)$. Also, two conditions are satisfied (see Appendix A).

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(i) $\mathcal{S}(\mathbb{R}_x)$ is an invariant subspace of $\hat{H}$.

(ii) $\hat{H}$ is continuous on $\mathcal{S}(\mathbb{R}_x)$.

The time-independent Schrödinger equation (1.7) is

$$-\frac{\hbar^2}{2m}\frac{d^2}{dx^2}u(x) + \left(V_0 - \frac{1}{2}m\gamma^2 x^2\right)u(x) = Eu(x). \tag{2.3}$$

It is convenient to introduce the dimensionless variables

$$\xi \equiv \beta x, \quad \beta \equiv \sqrt{\frac{m\gamma}{\hbar}}, \tag{2.4}$$

$$\lambda \equiv \frac{2(E - V_0)}{\hbar\gamma}. \tag{2.5}$$

Equation (2.3) now becomes

$$\frac{d^2u}{d\xi^2} + \left(\lambda + \xi^2\right)u = 0. \tag{2.6}$$

Step 1. The asymptotic solutions

We shall now obtain the asymptotic solutions of equation (2.6). If we neglect λ in (2.6) altogether, approximate solutions for large $|\xi|$ are

$$u^{\pm}(\xi) \approx \xi^n e^{\pm i\xi^2/2}, \tag{2.7}$$

where n is an arbitrary number. Substituting (2.7) into (2.6), we see that *the values $E^{\pm}$ of (2.5) associated with $u^{\pm}$ are complex numbers*:

$$E^+ \in \mathbb{C}_-, \quad E^- \in \mathbb{C}_+,$$

where the symbols $\mathbb{C}_{\pm}$ have the meaning

$$\mathbb{C}_{\pm} \equiv \{z = x + iy \mid x \in \mathbb{R}, \quad y \in \mathbb{R}_{\pm}\},$$
$$\mathbb{R}_+ \equiv [0, +\infty), \quad \mathbb{R}_- \equiv (-\infty, 0].$$

Since $\hat{H}$ is an essentially self-adjoint on $\mathcal{S}(\mathbb{R}_x)$, $u^{\pm}$ do not belong to a Lebesgue space $L^2(\mathbb{R}_x)$. For such eigenfunctions of $\hat{H}$ belonging to the complex energy eigenvalues, one can use the Gel'fand triplet which is formed by the Schwartz space $\mathcal{S}(\mathbb{R}_x)$ as a nuclear space [4, 7],

$$\mathcal{S}(\mathbb{R}_x) \subset L^2(\mathbb{R}_x) \subset \mathcal{S}(\mathbb{R}_x)^{\times}. \tag{2.8}$$

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Let us treat the extension $\hat{H}^\times$ of the Hamiltonian to the conjugate space $\mathcal{S}(\mathbb{R}_x)^\times$. We should be able to apply it to a generalized function $u \in \mathcal{S}(\mathbb{R}_x)^\times$, the product $\hat{H}^\times u$ being defined by [4, 7]

$$\left\langle v \,\middle|\, \hat{H}^\times u \right\rangle = \left\langle \hat{H}v \,\middle|\, u \right\rangle$$

for all functions $v \in \mathcal{S}(\mathbb{R}_x)$. Taking the x-representatives, we get

$$\int_{-\infty}^{\infty} v(x)^* \big(\hat{H}^\times u\big)(x) dx = \int_{-\infty}^{\infty} \big(\hat{H}v\big)(x)^* u(x) dx.$$

We can transform the right-hand side by partial integration and get

$$\int_{-\infty}^{\infty} v(x)^* \big(\hat{H}^\times u\big)(x) dx = \int_{-\infty}^{\infty} v(x)^* \big(\hat{H}u\big)(x) dx,$$

since v is a rapidly decreasing function, the contributions from the limits of integration vanish. This gives

$$\left\langle v \,\middle|\, \hat{H}^\times u \right\rangle = \left\langle v \,\middle|\, \hat{H}u \right\rangle,$$

showing that

$$\hat{H}^\times u = \hat{H}u.$$

Thus $\hat{H}^\times$ operating to a generalized function has the meaning of $\hat{H}$ operating.

The asymptotic solutions (2.7) will then be generalized functions or tempered distributions in $\mathcal{S}(\mathbb{R}_x)^\times$. We may verify that $u^\pm \in \mathcal{S}(\mathbb{R}_x)^\times$ by the Gauss-Fresnel integral, e.g. for any $x^m e^{-\alpha^2 x^2/2} \in \mathcal{S}(\mathbb{R}_x)$ $(m \in \mathbb{Z}_+, \alpha \in \mathbb{R})$,

$$\int_{-\infty}^{\infty} \left(x^m e^{-\alpha^2 x^2/2} \right)^* x^n e^{\pm i\beta^2 x^2/2} dx = (m+n-1)!! \sqrt{\frac{2\pi}{(\alpha^2 \mp i\beta^2)^{m+n+1}}}$$

when $m+n$ is even and zero otherwise.

Let us examine physical properties of the asymptotic states. The result of the momentum operator $\hat{p}^\times = -i\hbar d/dx$ applied to asymptotic solutions (2.7) is

$$-i\hbar \frac{d}{dx} u^\pm(x) \approx \pm \hbar\beta^2 x u^\pm(x). \tag{2.9}$$

Thus $u^+(x)$ represents particles moving outward to the infinity $x = \infty$, and $u^-(x)$ represents particles moving inward to the origin $x = 0$. We shall see in § 3.1 that this *space boundary condition* is justified by the asymptotic behaviors of the probability currents.

Step 2. The method of power series expansion

We shall work out the whole solutions of equation (2.6) by the method of power series expansion from (2.7). Put

$$u^\pm(\xi) = e^{\pm i\xi^2/2} H^\pm(\xi), \tag{2.10}$$

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introducing two new functions $H^{\pm}(\xi)$. Equation (2.6) becomes

$$\frac{d^2 H^{\pm}}{d\xi^2} \pm 2i\xi \frac{dH^{\pm}}{d\xi} + \left(\lambda^{\pm} \pm i\right) H^{\pm} = 0. \tag{2.11}$$

We now look for a solution of these equations in the form of power series[1]

$$H^{\pm}(\xi) = \xi^s \sum_{n=0}^{\infty} c_n^{\pm} \xi^n \quad \left(c_0^{\pm} \neq 0\right), \tag{2.12}$$

in which values of the leading order s need not be integers. Substituting (2.12) in (2.11) and picking out coefficients of ξ^n, we obtain

$$\left. \begin{array}{r} s(s-1)c_0^{\pm} = 0, \\ (s+1)s c_1^{\pm} = 0, \\ (s+n+2)(s+n+1)c_{n+2}^{\pm} = \left[\mp i(2s+2n+1) - \lambda^{\pm}\right] c_n^{\pm}. \end{array} \right\} \tag{2.13}$$

From the indicial equations of (2.13)

$$s = 0 \text{ or } 1. \tag{2.14}$$

We can investigate the convergence of the series (2.12) on the same lines as the harmonic oscillator. The third of equations (2.13) give approximately, when n is large,

$$\frac{c_{n+2}^{\pm}}{c_n^{\pm}} \approx \mp i \frac{2}{n}.$$

The series (2.12) will therefore converge like

$$H^{\pm}(\xi) \approx e^{\mp i\xi^2}$$

for large values of $|\xi|$. Thus, from (2.10), we have

$$u^{\pm}(\xi) \approx e^{\mp i\xi^2/2}.$$

These results change the asymptotic behaviors in which $u^{+}(\xi)$ goes off to infinity and $u^{-}(\xi)$ arrives from infinity. There are therefore in general no permissible solutions of (2.3) for which the series (2.12) extend to infinity on the side of large n. The permissible solutions, which satisfy the space boundary condition, arise when the series (2.12) terminate on the side of large n. The conditions for this termination of the series are

$$c_1^{\pm} = 0 \tag{2.15}$$

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[1]One cannot infer that $u^{\pm}(\xi)$ have a definite parity in this step, even though the potential energy of (2.1) is a symmetrical of ξ, since $u^{\pm}(\xi)$ are generally degenerate [2, 3].

and

$$\lambda^\pm = \mp i(2s + 2m + 1) \tag{2.16}$$

for some even m. In this case we get, from the recurrence formulas of (2.13),

$$c_1^\pm = c_3^\pm = \cdots = c_{m-1}^\pm = c_{m+1}^\pm = c_{m+2}^\pm = \cdots = 0.$$

Thus $H^\pm(\xi)$ are the polynomials of degree $s + m$. Since the only possible values of s are 0 or 1, we obtain from (2.16), by putting $s + m = n$,

$$E_n^\pm = V_0 \mp i \left(n + \frac{1}{2} \right) \hbar\gamma \in \mathbb{C}_\mp \quad (n = 0, 1, 2, \cdots). \tag{2.17}$$

This formulas give the *complex energy eigenvalues* for the parabolic potential barrier. For generalized eigenstates of $\hat{H}$ belonging to the generalized eigenvalues $E_n^\pm$, the time-independent wave functions are

$$u_n^\pm(x) = B_n^\pm e^{\pm i\beta^2 x^2/2} H_n^\pm(\beta x) \in \mathcal{S}(\mathbb{R}_x)^\times, \tag{2.18}$$

where $H_n^\pm(\beta x)$ are the polynomials of degree n (see Appendix B), and $B_n^\pm$ are the numerical coefficients. These numerical coefficients cannot be determined by the normalizing condition (1.9), since a scalar product of generalized functions is not defined. In general, a generalized function is not necessarily normalized [7]. However we can determine $B_n^\pm$ with the help of the following argument. Comparing above results with (A.6) and (A.7), we see that $E_n^\pm$ and $u_n^\pm(x)$ are the same form as in the harmonic oscillator from the analytical continuation (2.2) (see Appendix A). From (A.8), we therefore determine that

$$B_n^\pm = \left(\frac{\beta}{(\pm 2i)^n n! \sqrt{\pm i\pi}} \right)^{\frac{1}{2}} \tag{2.19}$$

with the correction from our definition of $H_n^\pm(\beta x)$ of Appendix B.

Let us now see the properties of time-independent wave functions under a space inversion. Property (B.3) of Appendix B shows that $u_n^\pm(x)$ are eigenstates of the parity,

$$u_n^\pm(-x) = (-)^n u_n^\pm(x).$$

The validity of this result depends on the space boundary condition.

The above results suggest that the eigenfunctions of the parabolic potential barrier are *non-stationary states.* It is obvious physically that the observational energy spectrum of this system is real and continuous. But the energy eigenvalues (2.17) are complex and discrete. The connection between the real continuous spectrum of observed energies and the complex discrete eigenvalues of mathematical eigenvalue problem will be dealt with in § 3.2.

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2.2　The momentum representation

The coordinate and the momentum representatives of a good function $f \in \mathcal{S}(\mathbb{R}_x)$ are connected by the Fourier transformations [1]

$$\left.\begin{aligned}
\tilde{f}(p) &= \left(\hat{\mathcal{F}}f\right)(p) \equiv \frac{1}{\sqrt{2\pi\hbar}} \int_{-\infty}^{\infty} f(x)e^{-ipx/\hbar}dx, \\
f(x) &= \left(\hat{\mathcal{F}}^{-1}\tilde{f}\right)(x) \equiv \frac{1}{\sqrt{2\pi\hbar}} \int_{-\infty}^{\infty} \tilde{f}(p)e^{ipx/\hbar}dp.
\end{aligned}\right\} \tag{2.20}$$

Let us treat the extension $\hat{\mathcal{F}}^{\times}$ of the Fourier transformation to the conjugate space $\mathcal{S}(\mathbb{R}_x)^{\times}$. We should be able to apply it to a generalized function $u \in \mathcal{S}(\mathbb{R}_x)^{\times}$, the product $\hat{\mathcal{F}}^{\times}u$ being defined by [4, 7, 8]

$$\left\langle v \,\middle|\, \hat{\mathcal{F}}^{\times}u \right\rangle = \left\langle \hat{\mathcal{F}}^{-1}v \,\middle|\, u \right\rangle$$

for all functions $v \in \mathcal{S}(\mathbb{R}_x)$. Taking the representatives, we get

$$\int_{-\infty}^{\infty} \tilde{v}(p)^* \left(\hat{\mathcal{F}}^{\times}u\right)(p)dp = \int_{-\infty}^{\infty} \left(\hat{\mathcal{F}}^{-1}\tilde{v}\right)(x)^* u(x)dx.$$

We can transform the right-hand side by the second of equations (2.20) and get

$$\int_{-\infty}^{\infty} \tilde{v}(p)^* \left(\hat{\mathcal{F}}^{\times}u\right)(p)dp = \int_{-\infty}^{\infty} \tilde{v}(p)^* \left(\hat{\mathcal{F}}u\right)(p)dp,$$

with the exchange of the order of the integrals by Fubini's theorem. This gives

$$\left\langle v \,\middle|\, \hat{\mathcal{F}}^{\times}u \right\rangle = \left\langle v \,\middle|\, \hat{\mathcal{F}}u \right\rangle,$$

showing that

$$\hat{\mathcal{F}}^{\times}u = \hat{\mathcal{F}}u.$$

Thus $\hat{\mathcal{F}}^{\times}$ operating to a generalized function has the meaning of $\hat{\mathcal{F}}$ operating.

We note that the Fourier transformation and its extension applied to (2.8) give a new Gel'fand triplet

$$\begin{array}{ccccc}
\mathcal{S}(\mathbb{R}_x) & \subset & L^2(\mathbb{R}_x) & \subset & \mathcal{S}(\mathbb{R}_x)^{\times} \\
\hat{\mathcal{F}} \downarrow & & \hat{\mathcal{F}} \downarrow & & \downarrow \hat{\mathcal{F}}^{\times} \\
\mathcal{S}(\mathbb{R}_p) & \subset & L^2(\mathbb{R}_p) & \subset & \mathcal{S}(\mathbb{R}_p)^{\times},
\end{array} \tag{2.21}$$

which is a unitary equivalent to (2.8) [4, 7, 8]. Written in terms of p-representatives, the Hamiltonian (2.1) gives

$$\hat{\mathcal{F}}\hat{H}\hat{\mathcal{F}}^{-1} = \frac{p^2}{2m} + V_0 + \frac{1}{2}m\gamma^2\hbar^2 \frac{d^2}{dp^2}, \tag{2.22}$$

an essentially self-adjoint on $\mathcal{S}(\mathbb{R}_p)$, and also the two conditions (i) and (ii) of § 2.1 are satisfied. For generalized eigenstates of (2.22) belonging to the generalized eigenvalues $E_n^\pm$, the time-independent wave functions are

$$\tilde{u}_n^\pm(p) = \tilde{B}_n^\pm e^{\mp i\tilde{\beta}^2 p^2/2} H_n^\mp(\tilde{\beta}p) \in \mathcal{S}(\mathbb{R}_p)^\times, \tag{2.23}$$

$$\tilde{B}_n^\pm = (-i)^n \left(\frac{\tilde{\beta}}{(\mp 2i)^n n! \sqrt{\mp i\pi}} \right)^{\frac{1}{2}}, \quad \tilde{\beta} \equiv \frac{1}{\sqrt{m\gamma\hbar}}. \tag{2.24}$$

Note that the phase factor $(-i)^n$ appears as a result of the Fourier transformations of $H_n^\pm$.

3 Motion in the parabolic potential barrier

3.1 The time evolution

Our work in § 2 has been concerned with one instant of time. The present section will be devoted to the variation with time of the non-stationary states.

We can get the time factors $T_n^\pm(t)$ corresponding to the complex energy eigenvalues $E_n^\pm$ by substituting (2.17) into (1.6). They give

$$T_n^\pm(t) = A_n^\pm e^{-iV_0 t/\hbar} e^{\mp(n+1/2)\gamma t}, \tag{3.1}$$

where $A_n^\pm$ are the numerical coefficients. The time-dependent wave functions $\psi_n^\pm(t, x)$ representing a non-stationary states of complex energy eigenvalues $E_n^\pm$ are, according to (1.5),

$$\begin{aligned}
\psi_n^\pm(t, x) &= T_n^\pm(t) u_n^\pm(x) \\
&= A_n^\pm B_n^\pm e^{-iV_0 t/\hbar} e^{\mp(n+1/2)\gamma t} e^{\pm i\beta^2 x^2/2} H_n^\pm(\beta x).
\end{aligned} \tag{3.2}$$

Before proceeding to discuss the physical meanings of the time factors (3.1), we shall first verify the equation of continuity. From (3.2) we see now that the probability densities are

$$\begin{aligned}
\rho_n^\pm(t, x) &\equiv \left| \psi_n^\pm(t, x) \right|^2 \\
&= \left| A_n^\pm \right|^2 \left| B_n^\pm \right|^2 e^{\mp(2n+1)\gamma t} H_n^\mp(\beta x) H_n^\pm(\beta x)
\end{aligned} \tag{3.3}$$

and the probability currents are

$$\begin{aligned}
j_n^\pm(t, x) &\equiv \Re \left[\psi_n^\pm(t, x)^* \left(-i\hbar\partial\psi_n^\pm/\partial x \right)(t, x) \right] / m \\
&= \pm \left| A_n^\pm \right|^2 \left| B_n^\pm \right|^2 e^{\mp(2n+1)\gamma t} \\
&\quad \times \gamma \left\{ x H_n^\mp(\beta x) H_n^\pm(\beta x) \pm 2n\beta^{-1} \Im \left[H_n^\mp(\beta x) H_{n-1}^\pm(\beta x) \right] \right\}.
\end{aligned} \tag{3.4}$$

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Equations (3.3) and (3.4) depend on the time t which satisfy the equation of continuity

$$\frac{\partial}{\partial t}\rho_n^{\pm}(t,x) + \frac{\partial}{\partial x}j_n^{\pm}(t,x) = 0, \tag{3.5}$$

with the help of formulas (B.6) and (B.7) of Appendix B. Note that the numerical coefficients $A_n^{\pm}$ and $B_n^{\pm}$ do not affect the validity of (3.5).

We must examine how the probability currents $j_n^{\pm}(t,x)$ behave for large values of $|x|$. The second term in the {} brackets in (3.4) can be neglected as $|x| \to \infty$. We are left with

$$j_n^{\pm}(t,x) \approx \pm\, 2^{2n}\left|A_n^{\pm}\right|^2\left|B_n^{\pm}\right|^2 e^{\mp(2n+1)\gamma t}\gamma\beta^{2n}x^{2n+1}$$
$$\approx \pm\, e^{\mp(2n+1)\gamma t}x^{2n+1}.$$

These asymptotic behaviors of probability currents show that the index $+$ (ψ_n^+, u_n^+, etc.) means only outward moving particles and the index $-$ (ψ_n^-, u_n^-, etc.) means only inward moving particles. These asymptotic behaviors are the one assumed in § 2.1 for dealing with the space boundary condition.

Let us now examine how the probability densities $\rho_n^{\pm}(t,x)$ vary with time. From (3.3), $\rho_n^{\pm}(t,x)$ will tend to infinity as $t \to \mp\infty$. The result is a necessary consequence of the form of time-dependent wave functions (3.2). In any case the time-dependent wave functions $\psi_n^{\pm}(t,x)$ must not tend to infinity as $t \to \mp\infty$, or they will represent states that have no physical meaning. The way of escape from the difficulty lies in the domains of the time factors (3.1). We assume that $T_n^+(t)$ exists only on the future part, for which $t > 0$, and $T_n^-(t)$ exists only on the past part, for which $t < 0$, i.e.

$$T_n^+(t) = A_n^+ e^{-iV_0 t/\hbar}e^{-(n+1/2)\gamma t} \quad \text{when } t > 0,$$
$$T_n^-(t) = A_n^- e^{-iV_0 t/\hbar}e^{(n+1/2)\gamma t} \quad \text{when } t < 0.$$

These equations can be combined into the single equations

$$T_n^{\pm}(t) = A_n^{\pm} e^{-iV_0 t/\hbar}e^{\mp(n+1/2)\gamma t}\theta(\pm t), \tag{3.6}$$

where $\theta(t)$ is the Heaviside step function. We take the squares of the moduli of the time factors (3.6)

$$\left|T_n^{\pm}(t)\right|^2 = \left|A_n^{\pm}\right|^2 e^{\mp(2n+1)\gamma t}\theta(\pm t). \tag{3.7}$$

To interpret the result (3.7), we may suppose that the index $+$ (ψ_n^+, T_n^+, etc.) refer to the *states of decay* when $t > 0$, while the index $-$ (ψ_n^-, T_n^-, etc.) refer to the *states of growth* when $t < 0$. This condition expresses mathematically that

$$T_n^+(t) \in L_+^2(\mathbb{R}_t), \quad T_n^-(t) \in L_-^2(\mathbb{R}_t), \tag{3.8}$$

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where spaces $L^2_\pm(\mathbb{R}_t)$ are defined by

$$L^2_\pm(\mathbb{R}_t) \equiv \left\{ f \in L^2(\mathbb{R}_t) \,\middle|\, f(t) = 0 \ \text{a.e.} \ t \in \mathbb{R}_\mp \right\}. \tag{3.9}$$

This condition will be referred to as the *time boundary condition.*

These boundary conditions require that $\psi_n^-(t, x)$ represents the growing state lying on the past part together with only inward moving particle and $\psi_m^+(t, x)$ represents the decaying state lying on the future part together with only outward moving particle. We must now obtain the probability of a transition taking place from state ψ_n^- to state ψ_m^+ at time $t = 0$. This gives us the "selection rule" at time $t = 0$, and can be worked out from the following transition matrix elements

$$S_{mn} = \left\langle u_m^+ \,\middle|\, u_n^- \right\rangle \equiv \int_{-\infty}^{\infty} u_m^+(x)^* u_n^-(x) dx, \tag{3.10}$$

the last definition expresses $\left\langle u_m^+ \,\middle|\, u_n^- \right\rangle$ in terms of x-representatives. When we substitute for $u_n^\pm(x)$ their value given by (2.18), equation (3.10) gives

$$S_{mn} = \beta^{-1} B_m^{+\,*} B_n^- \int_{-\infty}^{\infty} H_m^+(\xi)^* H_n^-(\xi) e^{-i\xi^2} d\xi$$

with the help of (2.4). The right-hand side becomes, from an application of formula (B.8) of Appendix B,

$$S_{mn} = \delta_{mn} \tag{3.11}$$

with the help of (2.19). The transition matrix is then a unit matrix. This result expresses that the state ψ_n^- $(n = 0, 1, 2, \cdots)$ on the past part is connected with the state ψ_n^+ having the same label n on the future part. Thus our selection rule at time $t = 0$ is that only those transitions can take place in which the complex energy changes from E_n^- to E_n^+.

Our problem now is to obtain the numerical coefficients $A_n^\pm$ of (3.6). We shall distinguish between the growing state ψ_n^- and the decaying state ψ_n^+ of the unstable system, with the growth and decay processes governed independently each by its own probability law [1]. We shall require that *the total number of growing particles is equal to the total number of decaying particles*, i.e.

$$\int_{-\infty}^{0} \rho_n^-(t, x) dt = \int_{0}^{\infty} \rho_n^+(t, x) dt. \tag{3.12}$$

By substituting for $\rho_n^\pm$ here their values given by (3.3), we now see that this condition (3.12) is independent of x. Thus (3.12) provides the condition for the time factor. From (3.12) we can require *the normalizing condition for the time factor*, as in equation (1.11) of § 1

$$\int_{-\infty}^{0} \left| T_n^-(t) \right|^2 dt = \int_{0}^{\infty} \left| T_n^+(t) \right|^2 dt = 1. \tag{3.13}$$

If we now apply these conditions (3.13) to the time factors (3.6), we have

$$A_n^\pm = \sqrt{(2n+1)\gamma},$$ (3.14)

where the phase factors are chosen unity.[2]

Let us now apply the rules of (1.12) for the interpretation of time factors. We find that the expectation values of t for the states $\psi_n^\pm$ are

$$\begin{aligned}
\langle t \rangle_n^\pm &\equiv \int_{-\infty}^{\infty} t \left| T_n^\pm(t) \right|^2 dt \\
&= \left| A_n^\pm \right|^2 \int_{-\infty}^{\infty} t e^{\mp(2n+1)\gamma t} \theta(\pm t) dt \\
&= \pm \frac{1}{(2n+1)\gamma},
\end{aligned}$$ (3.15)

respectively. Again, we find

$$\begin{aligned}
\langle t^2 \rangle_n^\pm &\equiv \int_{-\infty}^{\infty} t^2 \left| T_n^\pm(t) \right|^2 dt \\
&= \left| A_n^\pm \right|^2 \int_{-\infty}^{\infty} t^2 e^{\mp(2n+1)\gamma t} \theta(\pm t) dt \\
&= \frac{2}{[(2n+1)\gamma]^2}.
\end{aligned}$$

Hence the positive square roots of the variance of t for the states $\psi_n^\pm$ are

$$\begin{aligned}
(\Delta t)_n^\pm &\equiv \sqrt{\left\langle \left(t - \langle t \rangle_n^\pm \right)^2 \right\rangle_n^\pm} \\
&= \sqrt{\langle t^2 \rangle_n^\pm - \left(\langle t \rangle_n^\pm \right)^2} \\
&= \frac{1}{(2n+1)\gamma}.
\end{aligned}$$ (3.16)

Thus $(\Delta t)_n^+$ is equal to $(\Delta t)_n^-$, since the probability densities $|T_n^+(t)|^2$ and $|T_n^-(t)|^2$ are symmetrical with respect to the center $t = 0$. We may call these quantities $(\Delta t)_n^\pm$ the *mean lifetimes*. Equations (3.16) inform us that *the mean lifetimes are quantized in the unstable system with the Hamiltonian* (2.1). These results are closely connected with Heisenberg's uncertainty relation between time and energy. This matter will be dealt with in the next section.

Let us return to the time-dependent wave functions (3.2). We shall verify finally a time reversal. By application of property (B.4) of Appendix B, we get

$$\psi_n^\pm(-t, x)^* = \psi_n^\mp(t, x),$$

---

[2]We choose these phase factors so that the time-dependent wave functions are simple forms under a time reversal.

with the help of (3.14) and also of equation (2.19). Similarly we have in the p-representation

$$\tilde{\psi}_n^\pm(-t, -p)^* = \tilde{\psi}_n^\mp(t, p),$$

since the phase factor in equation (2.24) and the parity of $H_n^\pm(\tilde{\beta}p)$ cancel out. We see in this way that a time reversal occurs resulting in the interchange of states on the future part and on the past part. It is known as the *reciprocity theorem* [2].

3.2   The energy distribution

The time factor and the *physical* energy dependence of a function $f \in L_\pm^2(\mathbb{R}_t)$ are connected by the inverse Fourier transformations

$$\left.\begin{aligned}
\tilde{f}(E) &= (\hat{\mathcal{F}}^{-1} f)(E) \equiv \frac{1}{\sqrt{2\pi\hbar}} \int_{-\infty}^{\infty} f(t) e^{iEt/\hbar} dt, \\
f(t) &= (\hat{\mathcal{F}} \tilde{f})(t) \equiv \frac{1}{\sqrt{2\pi\hbar}} \int_{-\infty}^{\infty} \tilde{f}(E) e^{-iEt/\hbar} dE,
\end{aligned}\right\} \tag{3.17}$$

since the theory of relativity puts physical energy in the same relation to time as momentum to coordinate (see equations (2.20)).

We must now evaluate the physical energy dependence $\tilde{T}_n^\pm(E)$ for the time factors (3.6), and obtain the probability density of them. We make use of the Paley-Wiener theorem, which states that the inverse Fourier transformation is a unitary mapping from $L_\pm^2(\mathbb{R}_t)$ onto $H_\pm^2$, i.e.

$$\hat{\mathcal{F}}^{-1} L_\pm^2(\mathbb{R}_t) = H_\pm^2, \tag{3.18}$$

H_+^2 denoting a Hardy space on the upper half-plane and H_-^2 denoting a Hardy space on the lower half-plane. If we apply the first of equations (3.17) to the time factors (3.6) and (3.8), we then have

$$\begin{aligned}
\tilde{T}_n^\pm(E) &= \frac{A_n^\pm}{\sqrt{2\pi\hbar}} \int_{-\infty}^{\infty} e^{i(E-V_0)t/\hbar} e^{\mp(n+1/2)\gamma t} \theta(\pm t) dt, \\
&= \frac{\pm i}{\sqrt{\pi}} \frac{\sqrt{(n+1/2)\hbar\gamma}}{E - V_0 \pm i(n+1/2)\hbar\gamma} \in H_\pm^2,
\end{aligned} \tag{3.19}$$

with the help of (3.14). Thus $\tilde{T}_n^+(E)$ has a simple pole at the point

$$V_0 - i(n+1/2)\hbar\gamma \in \mathbb{C}_-,$$

and $\tilde{T}_n^-(E)$ has a simple pole at the symmetrical point

$$V_0 + i(n+1/2)\hbar\gamma \in \mathbb{C}_+$$

with respect to the real axis. To obtain the original equations (3.6) we note that, from an application of the second of equations (3.17) to (3.19), the integral being taken along a large semicircle in the lower half-plane when $t > 0$ and in the upper half-plane when $t < 0$.

By taking the squares of the moduli of (3.19) respectively, we obtain

$$\left|\tilde{T}_n^-(E)\right|^2 = \left|\tilde{T}_n^+(E)\right|^2 = \frac{1}{\pi}\frac{(n+1/2)\hbar\gamma}{(E-V_0)^2 + [(n+1/2)\hbar\gamma]^2}. \tag{3.20}$$

These physical energy distributions are the *Breit-Wigner resonance formulas*, having the same resonance energy V_0 and the half-widths

$$\Gamma_n^\pm = \left(n + \frac{1}{2}\right)\hbar\gamma. \tag{3.21}$$

Specially, the quantity Γ_n^+ is what is sometimes called the *decay width*. Equations (3.21) inform us that *the half-widths are quantized in the unstable system with the Hamiltonian* (2.1). The integrals of (3.20) with respect to E are

$$\int_{-\infty}^{\infty}\left|\tilde{T}_n^-(E)\right|^2 dE = \int_{-\infty}^{\infty}\left|\tilde{T}_n^+(E)\right|^2 dE = 1, \tag{3.22}$$

corresponding to (3.13), so $\tilde{T}_n^\pm(E)$ *are normalized*.

Let us take the products of the mean lifetimes $(\Delta t)_n^\pm$ and the half-widths $\Gamma_n^\pm$. From (3.16) and (3.21) these products read

$$(\Delta t)_n^\pm \Gamma_n^\pm = \frac{\hbar}{2}. \tag{3.23}$$

These results are independent of n. *There are thus Heisenberg's uncertainty relations between the mean lifetimes and the half-widths.*

4 Discussion

We have obtained some insight into the main features of the unstable system by making a study of the one-dimensional parabolic potential barrier. The results of solving the time-independent Schrödinger equation for the unstable system are complex energy eigenvalues and generalized eigenfunctions in Gel'fand triplet. These generalized eigenfunctions are non-stationary states. We have assumed that the time factor corresponding to a non-stationary state is a square-integrable function. This assumption requires that the states of complex energy eigenvalues in the lower half-plane exist only on the future part and those of complex energy eigenvalues in the upper half-plane exist only on the past part. They correspond to the states of decay and growth, respectively. The distributions of physical energy of these decaying and growing states are given by the Breit-Wigner resonance

formulas whose half-widths are determined by the complex energy eigenvalues. Thus the half-widths are quantized in the unstable system instead that the values of physical energy are quantized in the stable system (e.g. the harmonic oscillator, the hydrogen atom). These results are capable of comparison with experiments. The observational results will provide a confirmation of the complex energy eigenvalues and generalized eigenfunctions in Gel'fand triplet.

We may discuss the comparison with the formulation given by Bohm and Gadella [4]. According to their formulation Gamow vectors (i.e. the states of resonance corresponding to a pair of simple poles of the S-matrix) are represented by generalized functions of the following Gel'fand triplets,

$$
\begin{array}{ccccc}
\mathcal{S}_{\pm}(\mathbb{R}_t) & \subset & L^2_{\pm}(\mathbb{R}_t) & \subset & \mathcal{S}_{\pm}(\mathbb{R}_t)^{\times} \\
\hat{\mathcal{F}}^{-1} \downarrow & & \hat{\mathcal{F}}^{-1} \downarrow & & \downarrow (\hat{\mathcal{F}}^{-1})^{\times} \\
\Delta_{\pm} & \subset & H^2_{\pm} & \subset & \Delta_{\pm}^{\times},
\end{array}
$$

where $\mathcal{S}_{\pm}(\mathbb{R}_t) \equiv \mathcal{S}(\mathbb{R}_t) \cap L^2_{\pm}(\mathbb{R}_t)$ and $\Delta_{\pm} \equiv \mathcal{S}(\mathbb{R}_E) \cap H^2_{\pm}$. The time evolution on $\Delta_{+}^{\times}$ is well defined only on the future part and that on $\Delta_{-}^{\times}$ is well defined only on the past part. We could, however, express the time factor as a Hilbert vector (§ 3), while we described the time-independent wave function by Gel'fand triplets (§ 2). We thus see that the origin of the separation of the domain of the time evolution lies in the property of the square-integrable of the time factor.

In §§ 3.1 and 3.2 we supposed that there is no interference between the growth and decay processes. In dealing with these processes, a further possibility to be taken into consideration is the direct scattering [1]. In this case, we must first require *the continuity condition for the time factor at time $t = 0$*

$$
T_n^-(0) = T_n^+(0). \tag{4.1}
$$

The reason for this condition (4.1) is that the time-dependent Schrödinger equation (1.1) is linear in the operator $\partial/\partial t$. We can now require *the normalizing condition for the time factor*, instead of (3.13)

$$
\int_{-\infty}^{\infty} \left| T_n^-(t) + T_n^+(t) \right|^2 dt = 1. \tag{4.2}
$$

This condition (4.2) means that the total probability of the state n being at any time is unity. The total energy dependence, namely $\tilde{T}_n^-(E)$ plus $\tilde{T}_n^+(E)$, is a real function of E. By taking the square of the modulus of the sum, we obtain

$$
\left| \tilde{T}_n^-(E) + \tilde{T}_n^+(E) \right|^2 = \frac{2}{\pi} \frac{[(n + 1/2)\hbar\gamma]^3}{\{(E - V_0)^2 + [(n + 1/2)\hbar\gamma]^2\}^2} \tag{4.3}
$$

Comparing this with (3.20), we see that the distribution (4.3) has a narrow width (its quarter-width is equal to $\Gamma_n^{\pm}$ given by (3.21)) and a sharp peak (its maximum value is

twice that of (3.20)) at the same point $E = V_0$. This distribution is different from the Breit-Wigner resonance formula. It is necessary to re-examine experimental data of an absorption line induced by the scattering process. We will investigate how this difference would appear experimentally.

The foregoing work shows how the properties of the time factor of the non-stationary state (of the unstable system) are similar to the properties of the time-independent wave function of the bound state (of the stable system), and vice versa. Further, the physical energy of the unstable system is the continuous spectrum running from $-\infty$ to ∞, and the lowest energy does not exist. We should thus expect to find *time operators* for the unstable system in quantum mechanics. The subject for further investigation is to get these time operators and set up a relativistic quantum mechanics treating the time and coordinates *as observables* on the same footing.

Appendices

A   The harmonic oscillator

The Hamiltonian of the one-dimensional harmonic oscillator is

$$\hat{H} = -\frac{\hbar^2}{2m}\frac{d^2}{dx^2} + V_0 + \frac{1}{2}m\omega^2 x^2, \tag{A.1}$$

where $V_0 \in \mathbb{R}$ is the minimum potential energy, $m > 0$ is the mass and $\omega > 0$ is the angular frequency. This Hamiltonian is an essentially self-adjoint on a Schwartz space $\mathcal{S}(\mathbb{R}_x)$. Further, two conditions are satisfied [4, 7].

(i) $\mathcal{S}(\mathbb{R}_x)$ is an invariant subspace of $\hat{H}$.

(ii) $\hat{H}$ is continuous on $\mathcal{S}(\mathbb{R}_x)$.

The time-independent Schrödinger equation (1.7) is

$$-\frac{\hbar^2}{2m}\frac{d^2}{dx^2}u(x) + \left(V_0 + \frac{1}{2}m\omega^2 x^2\right)u(x) = Eu(x). \tag{A.2}$$

It is convenient to introduce the dimensionless variables

$$\xi \equiv \alpha x, \ \ \alpha \equiv \sqrt{\frac{m\omega}{\hbar}}, \tag{A.3}$$

$$\lambda \equiv \frac{2(E - V_0)}{\hbar\omega}. \tag{A.4}$$

Equation (A.2) now becomes

$$\frac{d^2u}{d\xi^2} + \left(\lambda - \xi^2\right)u = 0. \tag{A.5}$$

Under the boundary condition $u \in \mathcal{S}(\mathbb{R}_x)$, this equation can be solved by the method of power series expansion. The energy eigenvalues are

$$E_n = V_0 + \left(n + \frac{1}{2} \right) \hbar\omega \in \mathbb{R} \quad (n = 0, 1, 2, \cdots) \tag{A.6}$$

and the eigenfunctions are

$$u_n(x) = N_n e^{-\alpha^2 x^2/2} H_n(\alpha x) \in \mathcal{S}(\mathbb{R}_x), \tag{A.7}$$

$$N_n = \left(\frac{\alpha}{2^n n! \sqrt{\pi}} \right)^{\frac{1}{2}}. \tag{A.8}$$

Here $H_n(\alpha x)$ are the Hermite polynomials of degree n, and the constants N_n are determined by the normalizing condition (1.9). The set of eigenfunctions $\{u_n\}_{n=0}^{\infty}$, given by (A.7), forms a complete orthonormal system on a Lebesgue space $L^2(\mathbb{R}_x)$ [8].

The energy eigenvalues (A.6) show that the probability densities of one-dimensional harmonic oscillator are time-independent, i.e. the eigenfunctions (A.7) are stationary states.

B Properties of the polynomials $H_n^{\pm}(\xi)$

The differential equations (2.11) with (2.16)

$$\frac{d^2 H_n^{\pm}}{d\xi^2} \pm 2i\xi \frac{dH_n^{\pm}}{d\xi} \mp 2in H_n^{\pm} = 0, \tag{B.1}$$

where $H_n^{\pm}(\xi)$ are the polynomials of degree n. If we define them so that the highest power of ξ appears with the coefficient 2^n, the first few polynomials calculated from (2.13) are

$$H_0^{\pm}(\xi) = 1, \quad H_1^{\pm}(\xi) = 2\xi, \quad H_2^{\pm}(\xi) = 4\xi^2 \mp 2i,$$
$$H_3^{\pm}(\xi) = 8\xi^3 \mp 12i\xi, \quad H_4^{\pm}(\xi) = 16\xi^4 \mp 48i\xi^2 - 12.$$

These polynomials in general can be expressed as

$$H_n^{\pm}(\xi) = (\mp i)^n \, e^{\mp i\xi^2} \frac{d^n}{d\xi^n} e^{\pm i\xi^2}. \tag{B.2}$$

Thus the parity of $H_n^{\pm}(\xi)$ is

$$H_n^{\pm}(-\xi) = (-)^n H_n^{\pm}(\xi), \tag{B.3}$$

and the conjugate complex of $H_n^{\pm}(\xi)$ is

$$H_n^{\pm}(\xi)^* = H_n^{\mp}(\xi). \tag{B.4}$$

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An alternative way of defining the polynomials $H_n^\pm(\xi)$ is as the generating functions $S^\pm(\xi, s)$ given by

$$S^\pm(\xi, s) \equiv e^{\mp i(2s\xi - s^2)} = \sum_{n=0}^\infty \frac{H_n^\pm(\xi)}{n!}(\mp is)^n. \tag{B.5}$$

From this definition we obtain the recurrence formulas

$$H_{n+1}^\pm - 2\xi H_n^\pm \pm 2in H_{n-1}^\pm = 0, \tag{B.6}$$

$$dH_n^\pm/d\xi = 2n H_{n-1}^\pm. \tag{B.7}$$

Corresponding to the orthogonality relation of the Hermite polynomials, we now have, from (B.5)

$$\int_{-\infty}^\infty H_m^\mp(\xi)^* H_n^\pm(\xi) e^{\pm i\xi^2} d\xi = (\pm 2i)^n n! \sqrt{\pm i\pi}\, \delta_{mn}, \tag{B.8}$$

where δ_{mn} is the Kronecker delta symbol.

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